A fresh computational approach to atomic structures and processes ... relevant for plasma & material physics

Stephan Fritzsche
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16th April 2018

Simple atomic processes:

$$A^* \longrightarrow A^{(*)} + \hbar\omega \qquad \text{... photon emission}$$

$$A + \hbar\omega \longrightarrow A^* \qquad \text{... photon excitation}$$

$$A + \hbar\omega \longrightarrow A^{+*} + e_p^-$$

$$A^{q+*} \longrightarrow A^{(q+1)+(*)} + e_a^-$$

$$e_s^- + A \longrightarrow A^* + e_s^{-\prime}$$

$$e_s^- + A \longrightarrow A^* + e_s^{-\prime} + e^-$$

$$A + n\,\hbar\omega \longrightarrow A^*$$

A fresh computational approach to atomic structures and processes ... relevant for plasma & material physics

Simple atomic processes:

$$A^* \longrightarrow A^{(*)} + \hbar\omega \quad \text{... photon emission}$$

$$A + \hbar\omega \longrightarrow A^* \quad \text{... photon excitation}$$

$$A + \hbar\omega \longrightarrow A^{+*} + e_p^- \quad \text{... (atomic) photoionization}$$

$$A^{q+*} \longrightarrow A^{(q+1)+(*)} + e_a^- \quad \text{... Auger emission; autoionization}$$

$$e_s^- + A \longrightarrow A^* + e_s^{-\prime} \quad \text{... electron - impact excitation}$$

$$e_s^- + A \longrightarrow A^* + e_s^{-\prime} + e^- \quad \text{... electron - impact ionization}$$

$$A + n\,\hbar\omega \longrightarrow A^* \quad \text{... multi - photon excitation/decay}$$

Quiz: Atomic processes in a nutshell

-- for “intermediates” in atomic and plasma physics

$$A + n\,\hbar\omega \longrightarrow A^{+(*)} + e_p^- \qquad \text{... multi-photon ionization}$$

$$A + n\,\hbar\omega \longrightarrow A^{+(*)} + (e_{p_1}^- + e_{p_2}^-) \qquad \text{... multi-photon double ionization}$$

$$A^{q+} + e_s^- \longrightarrow A^{(q-1)+} + \hbar\omega$$

$$A^{q+} + e_s^- \longrightarrow A^{(q-1)+*} \longrightarrow A^{(q-1)+(*)} + \hbar\omega$$

$$A + \hbar\omega \longrightarrow A^{(*)} + \hbar\omega'$$

$$A^{q+*} \longrightarrow A^{(q+1)+(*)} + (e_a^- + \hbar\omega)$$

$$A^{q+*} \longrightarrow A^{(q+2)+(*)} + (e_{a_1}^- + e_{a_2}^-)$$

$$A + \hbar\omega \longrightarrow A^* \longrightarrow A^{(*)} + \hbar\omega'$$

$$A + \hbar\omega \longrightarrow A^{+,*} + e_p^- \longrightarrow A^{(*)} + e_p^- + \hbar\omega'$$

$$A + Z_p \longrightarrow A^* + Z_p'$$

$$A^{(q+1)+} + Z_p \longrightarrow A^{(q+1)+(*)} + e^- + Z_p'$$

Quiz: Atomic processes in a nutshell

-- for “intermediates” in atomic and plasma physics

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$$A + n\,\hbar\omega \longrightarrow A^{+(*)} + (e_{p_1}^- + e_{p_2}^-) \quad \text{... multi-photon double ionization}$$

$$A^{q+} + e_s^- \longrightarrow A^{(q-1)+} + \hbar\omega \quad \text{... radiative recombination}$$

$$A^{q+} + e_s^- \longrightarrow A^{(q-1)+*} \longrightarrow A^{(q-1)+(*)} + \hbar\omega \quad \text{... dielectronic recombination}$$

$$A + \hbar\omega \longrightarrow A^{(*)} + \hbar\omega' \quad \text{... Rayleigh/Compton}$$

$$A^{q+*} \longrightarrow A^{(q+1)+(*)} + (e_a^- + \hbar\omega) \quad \text{... radiative Auger}$$

$$A^{q+*} \longrightarrow A^{(q+2)+(*)} + (e_{a_1}^- + e_{a_2}^-) \quad \text{... double Auger}$$

$$A + \hbar\omega \longrightarrow A^* \longrightarrow A^{(*)} + \hbar\omega' \quad \text{... photo-excitation \& fluorescence}$$

$$A + \hbar\omega \longrightarrow A^{+,*} + e_p^- \longrightarrow A^{(*)} + e_p^- + \hbar\omega' \quad \text{... photo-ionization \& fluorescence}$$

$$A + Z_p \longrightarrow A^* + Z_p' \quad \text{... Coulomb excitation}$$

$$A^{(q+1)+} + Z_p \longrightarrow A^{(q+1)+(*)} + e^- + Z_p' \quad \text{... Coulomb ionization}$$

- Indeed, these and many similar processes occur in atomic, plasma and astro physics as well as at many places elsewhere.
- How much help can atomic theory provide ? -- Which tools are available ?

Quiz: Atomic processes in a nutshell

-- for “intermediates” in atomic and plasma physics

$$A + n\,\hbar\omega \longrightarrow A^{+(*)} + e^-_p \quad \text{... multi-photon ionization}$$

$$A + n\,\hbar\omega \longrightarrow A^{+(*)} + (e^-_{p_1} + e^-_{p_2}) \quad \text{... multi-photon double ionization}$$

$$A^{q+} + e^-_s \longrightarrow A^{(q-1)+} + \hbar\omega \quad \text{... radiative recombination}$$

$$A^{q+} + e^-_s \longrightarrow A^{(q-1)+*} \longrightarrow A^{(q-1)+(*)} + \hbar\omega \quad \text{... dielectronic recombination}$$

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$$A^{q+*} \longrightarrow A^{(q+1)+(*)} + (e^-_a + \hbar\omega) \quad \text{... radiative Auger}$$

$$A^{q+*} \longrightarrow$$

$$A + \hbar\omega \longrightarrow$$

$$A + \hbar\omega \longrightarrow$$

$$A + Z_p \longrightarrow$$

$$A^{(q+1)+} + Z_p \longrightarrow$$

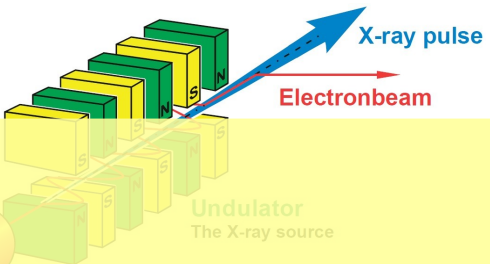
- Indeed, the
  physics a
- How much

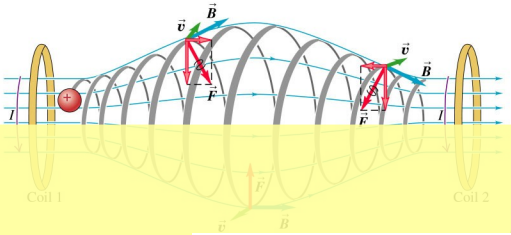
Plan of this talk

- Demands from experiment & theory: Two quick examples
- Established structure codes: Strength and weaknesses
- JAC: A fresh approach to atomic computations
- Amplitudes, properties & processes
- Atomic cascades
- Summary & conclusions

Demands for atomic theory

– to (accurately) describe the dynamics of many-electron systems





XUV- & XFEL's

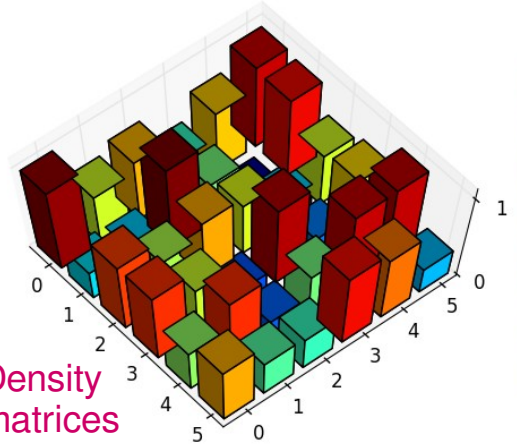
Undulator
The X-ray source

Laser pulse

Dirac's equation

$$(\beta mc^2 + c\vec{\alpha}.\vec{p})\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t}$$

Atomic QED techniques



Density matrices

$$\left\{-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial r_m^2}-\frac{l_i(l_i+1)}{r_m^2}\right]+\sum_{\mathbf{R}_i}\frac{-Ze^2}{|\mathbf{r}_m-\mathbf{R}_i|}\right\}P_i(r_m)$$
$$+\left[\sum_j^{occ}\int dr_n P_j^{\dagger}(r_n)\frac{e^2}{|r_m-r_n|}P_j(r_n)\right]P_i(r_m)$$
$$-\left[\sum_j^{occ}\int dr_n P_j^{\dagger}(r_n)\frac{e^2}{|\mathbf{r}_m-\mathbf{r}_n|}P_i(r_n)\right]P_j(r_m)=\varepsilon_i P_i(r_m)$$

Dirac-Fock & beyond

merge-beam experiments

ion traps

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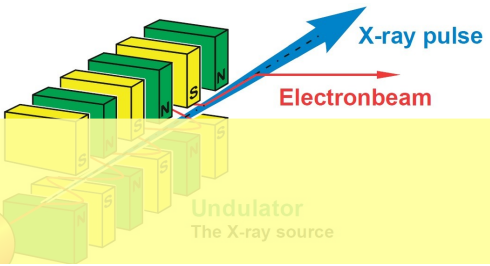

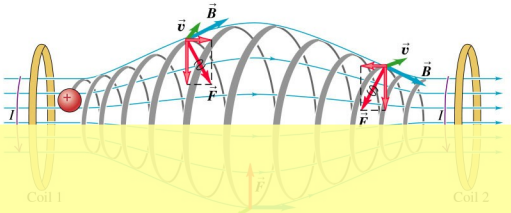

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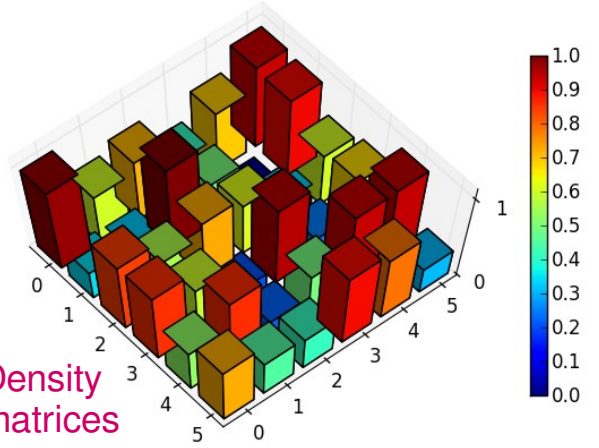

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Dirac-Fock & beyond

merge-beam experiments

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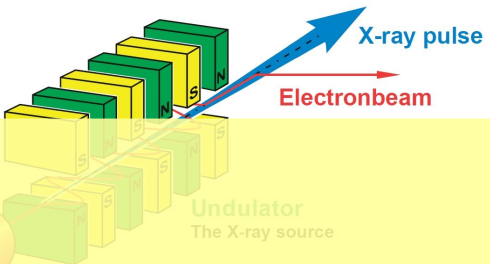
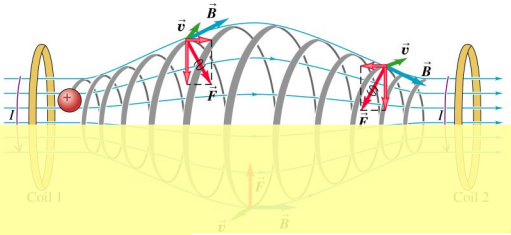
Demands for atomic theory

– to (accurately) describe the dynamics of many-electron systems





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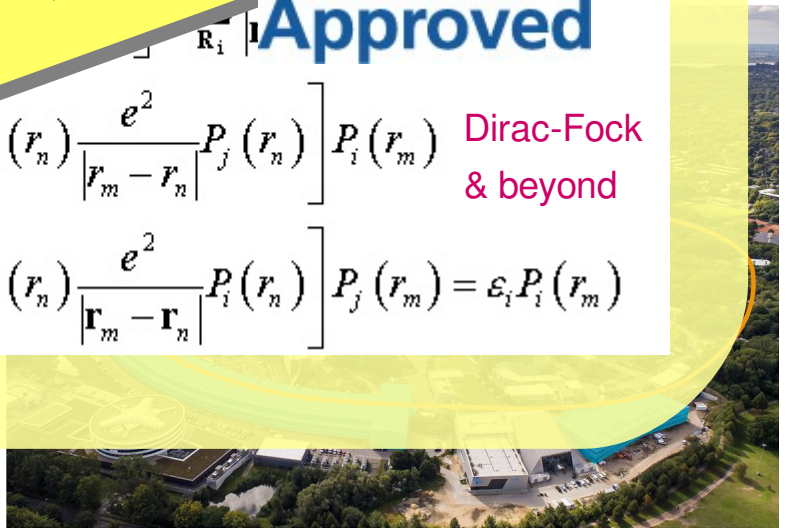
$$(\beta mc^2 + c\vec{\alpha}.\vec{p})\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t}$$

Accurate Atomic Amplitudes

$$\langle \Phi_\alpha \| V^L \| \Phi_\beta \rangle$$

Density matrices



$$\left[\sum_j \int dr_n P_j^\dagger(r_n)\frac{e^2}{|r_m - r_n|}P_j(r_n)\right]P_i(r_m)$$

$$-\left[\sum_j^{occ} \int dr_n P_j^\dagger(r_n)\frac{e^2}{|\mathbf{r}_m - \mathbf{r}_n|}P_i(r_n)\right]P_j(r_m) = \varepsilon_i P_i(r_m)$$

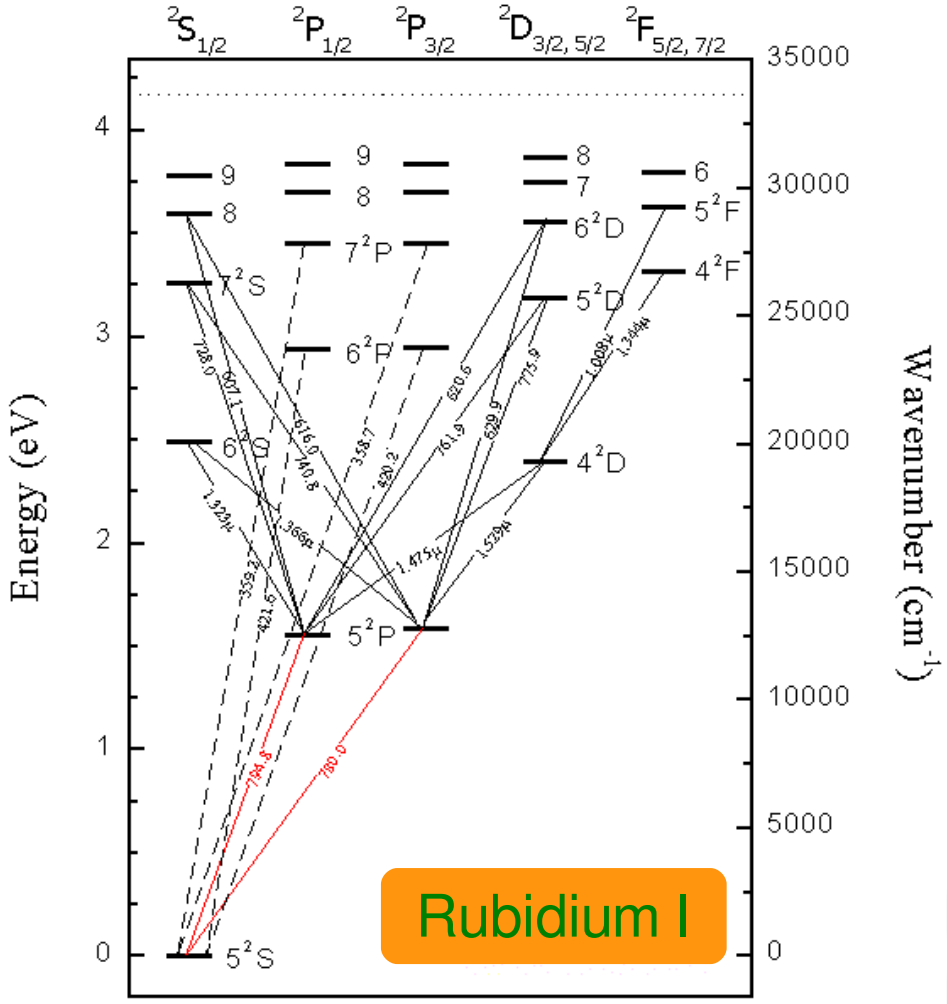
Dirac-Fock & beyond

Approved

ion traps

1 Level identification of atoms and ions

– Grotrian diagram as a unique finger print

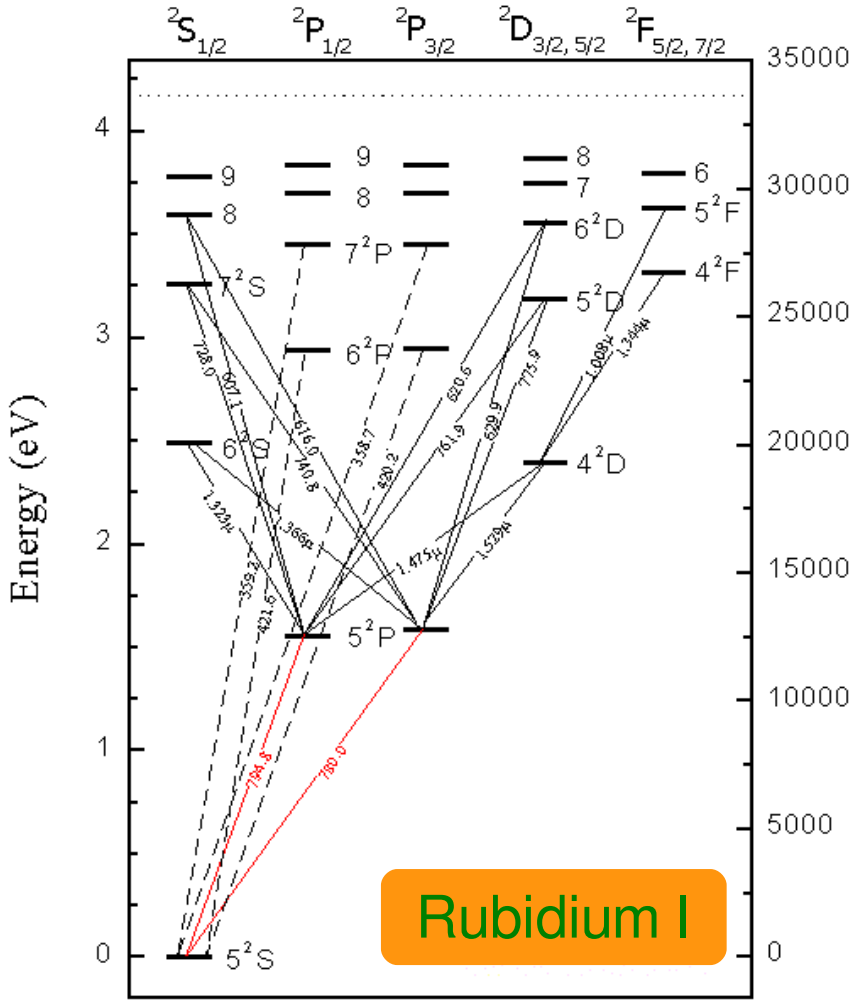


$4s^2\ 4p^6$ (5s + 5p + 4d + 6s + ...)

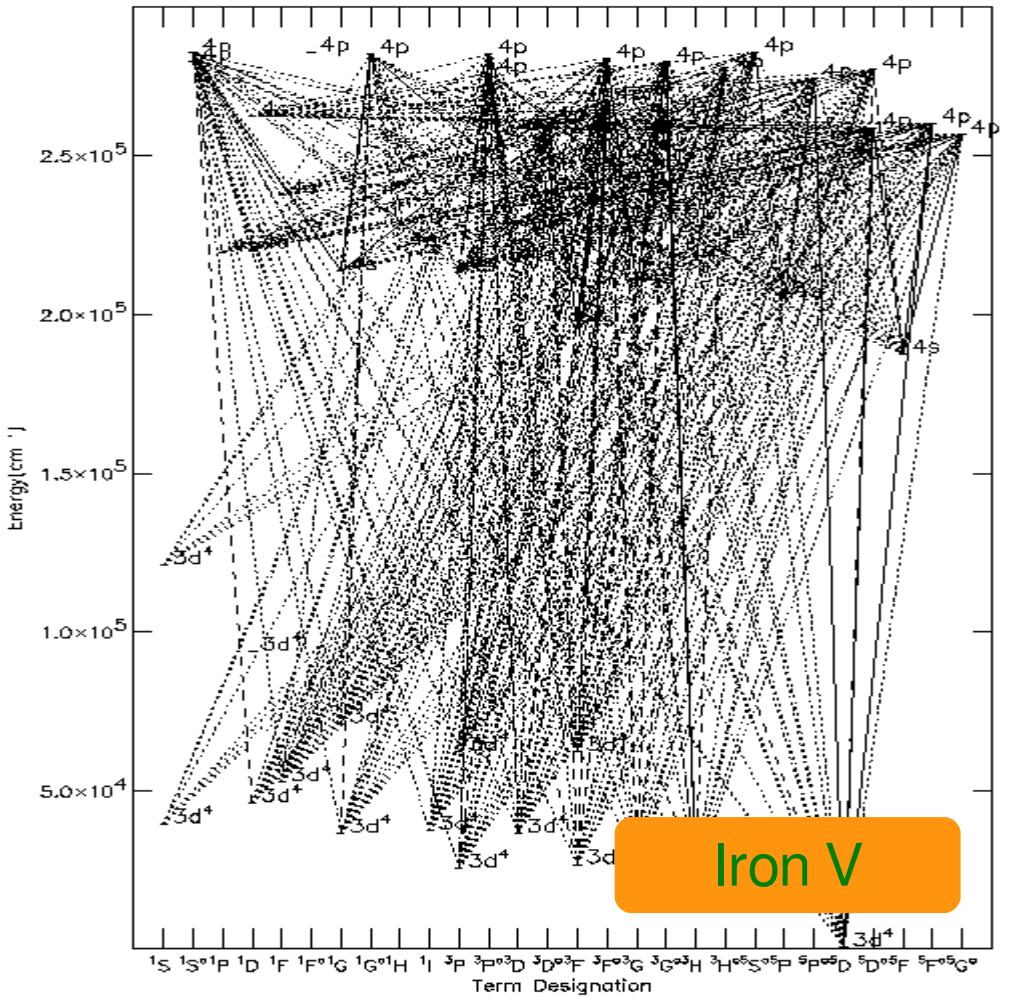
- Term diagrams: gross & fine structure.
- Allowed transitions and selection rules.
- Useful for one & multi-electron atoms.

1 Level identification of atoms and ions

– unique ... but often (very) complex



$4s^2\ 4p^6$ (5s + 5p + 4d + 6s + ...)



$3s^2\ 3p^6$ ($3d^4$ + ...)

1 Level identification of atoms and ions

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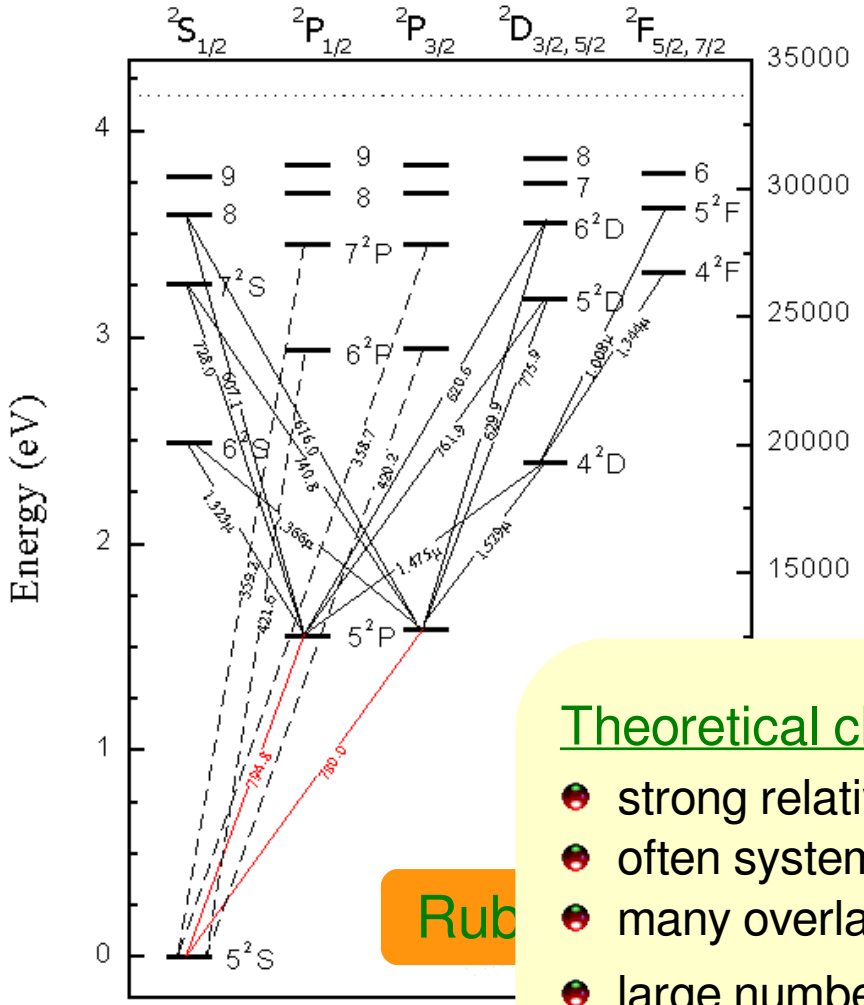
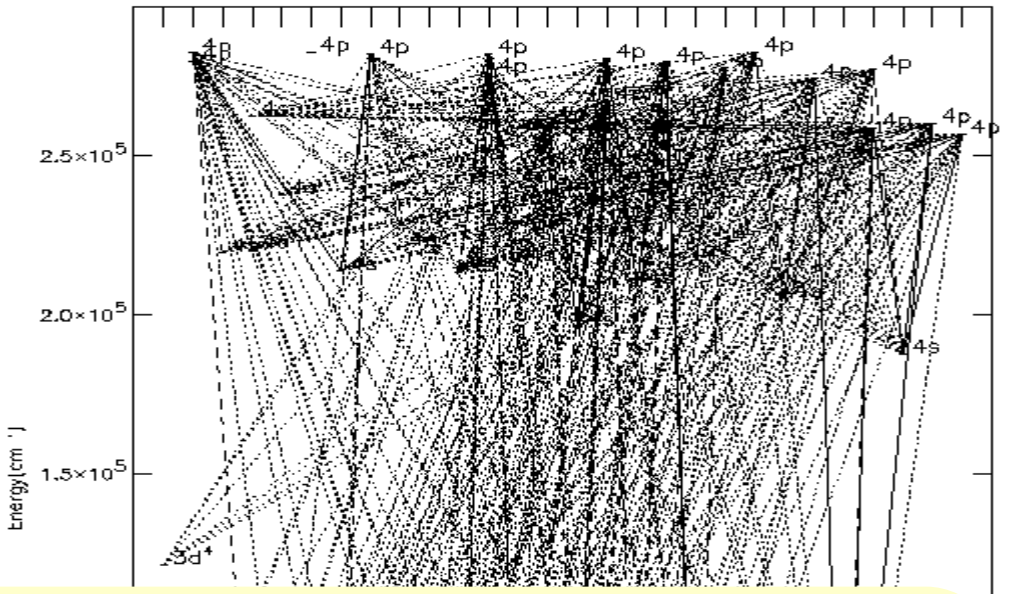




Rub

$4s^2\ 4p^6$ (5s + 5p + 4

Theoretical challenges for medium and heavy elements:

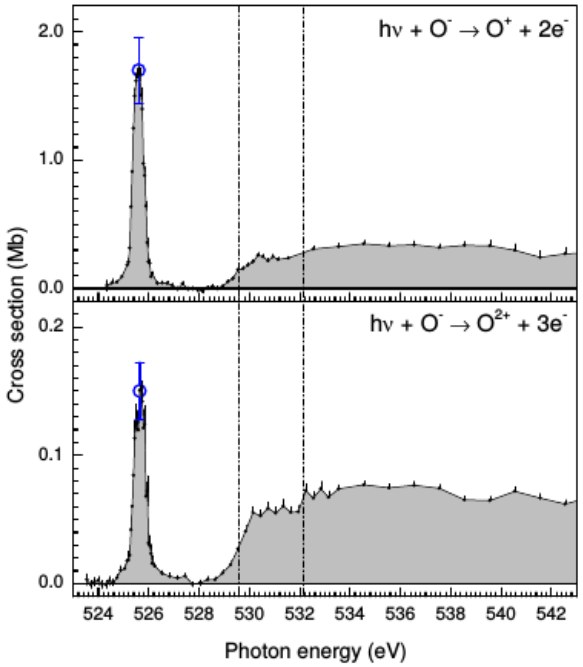
- strong relativistic and QED effects
- often systems with open d- and f-shells
- many overlapping and nearly degenerate configurations
- large number of electrons

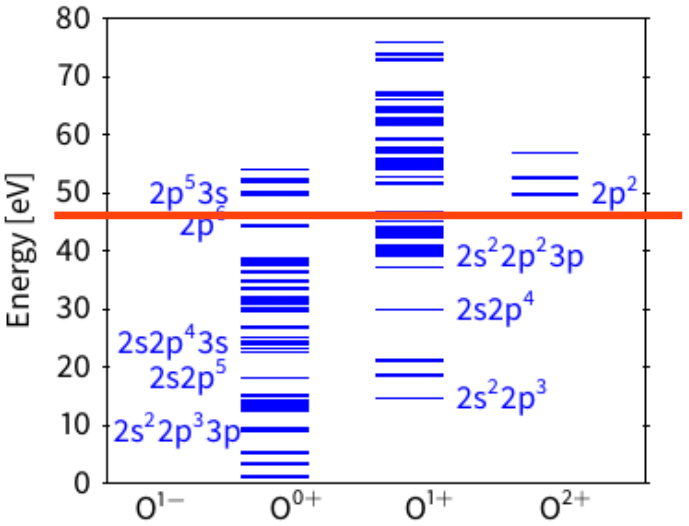
→ identification difficult or hardly feasible

2 Ion & electron spectra after inner-shell excitations

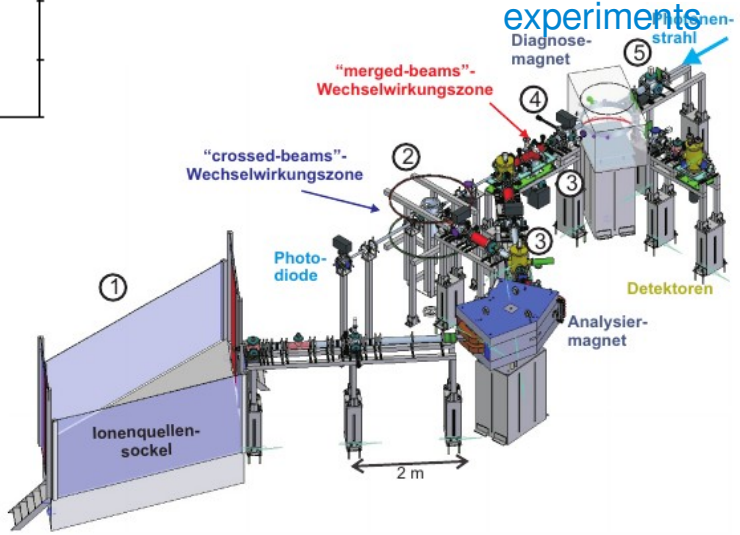
– 1s-2p excitation of O^-, recorded at PIPE

$$O^-(1s^2\,2s^2\,2p^5) + \gamma \rightarrow O^-(1s\,2s^2\,2p^6\ {}^2S_{1/2}) \rightarrow O^{(m-1)+}(1s^2\,2l^{7-m}) + m\,e^-$$





merge-beam experiments



Double & triple detachments by Auger electron emission are energetically forbidden.

→ possible only due to shake-up

2s → 3s, 2p → 3p

S. Schippers et al, PRA 94 (2016) 052412.

PIPE – Photon-Ion spectrometer at PETRA III (Hamburg)

S. Schippers and coworkers, Gießen, Frankfurt, Hamburg collaboration (2015).

Established tools for atomic-structure calculations

-- including great experience

- Clementi-Roetti: Roothan-Hartree-Fock wave functions with optimized exponents.
- Cowan's HFX: support & semi-empirical adjustment of level structures, transition probabilities & cross sections.
- ATSP: Breit-Pauli approximation, level energies & properties.
- Grasp/Ratip: Large-scale computations of individual energies, rates, ...
- FAC: Modelling and diagnostics of astro- & plasma processes.
  Flexible Atomic Code
- CI-MBPT: Combines CI and MBPT methods for bound-state properties.
- ...
- “Home-made”: Large No. of tools for particular purposes.

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... and with a **huge** number of applications
(and citations) from all fields of AMO & related physics

& plasma processes

ines CI and MBPT methods for bound-state properties.

S. Fritzsche, JESRP 114-116 (2001) 1155; Comput. Phys. Commun. 183 (2012) 1525

RATIP

Relativistic Atomic Transition, Ionization and Recombination Properties

AUGER: Auger rates, relative intensities, angular distribution & spin polarization parameters.

CESD: Determinant representation of atomic and configuration state functions.

REC: Radiative recombination & electron capture rates, angular parameters.

RELCI: Relativistic configuration interaction wave functions & QED estimates.

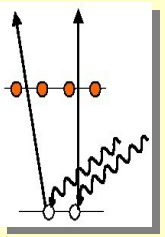
REOS: Relaxed-orbital Einstein A and B coefficients, transition probabilities and lifetimes.

TOOLBOX: Level energies and notations; manipuations of file interfaces, miscelaneous.

COULOMB: Exitation amplitudes, (M_J-dependent) cross sections, alignment parameters.

Many-electron basis (wave function expansions)

- Construction and classification of N-particle Hilbert spaces
- Shell model: Systematically enlarged CSF basis
- Interactions
  - Dirac-Coulomb Hamiltonian
  - Breit interactions + QED
  - Electron continuum; scattering phases
- Coherence transfer and Rydberg dynamics



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- ...
- "Home-made": Large No. of tools for particular purposes.

Most often, Fortran (or C, C++) codes ... quite technical & with little use of the underlying 'physics language' as developed in atomic theory; difficult to extent towards new processes, coding is typically cumbersome.

Quiz: Atomic processes in a nutshell

-- and now for the “experts”

$$A + \hbar\omega \longrightarrow A^* \longrightarrow A^{(*)} + e_a^-$$ ... photo – excitation autoionization

$$A + e_s^- \longrightarrow A^* + e_s^{-\prime} \longrightarrow A^{+(*)} + e_s^{-\prime} + e_a^-$$ ... impact – excitation autoionization

$$A + \hbar\omega \longrightarrow A^{+,*} + e_p^- \longrightarrow A^{(*)} + e_p^- + e_a^-$$ ... photo – ionization autoionization

$$A + \hbar\omega + \hbar\omega' \longrightarrow A^* + \hbar\omega' \longrightarrow A^{+*} + e_p^-$$ ... resonant 2 – color ionization

$$A^{q+} + e_s^- \longrightarrow A^{(q-1)+*} \longrightarrow A^{q+*} + e_{a_1}^- \longrightarrow A^{(q+1)+} + e_{a_1}^- + e_{a_2}^-$$ ... REDA

$$A^{q+} + e_s^- \longrightarrow A^{(q-1)+*} \longrightarrow A^{(q+1)+} + (e_{a_1}^- + e_{a_2}^-)$$ ... READI

$$A^{q+} + \hbar\omega \longrightarrow A^{(q-1)+*} + e^+$$ ... e^+ e^- (bound) pair production

$$A^{q+} + e^+ \longrightarrow A^{(q+1)+*} + \hbar\omega$$ ... e^+ e^- (bound) pair annihilation

$$A^{q+} + e_s^- \longrightarrow A^{(q-2)+*} + e^+$$ ... negative – continuum DR

Jena's Atomic Calculator (JAC)

-- A fresh approach to the computation of atoms, ...

JAC ... Jena's atomic calculator provides tools for performing atomic (structure) calculations at various degrees of complexity and sophistication.

What do we need in atomic structure and collision theory ?

- Design of a high-level language with data types close to atomic physics.

  Shell, Subshell, Configuration, Orbital, Basis, Level, Multiplet, Cascade, Pulse, ...

- Implementation and comparison of different models & approximations.
- Simple to learn and apply.

  With a simplified control; standard vs. advanced computations, complete active spaces; atomic cascades; ...

- Simple access to graphical interfaces and representations.
- Support a coarse-grained decomposition of most computational steps.

  A pseudo-code description should allow summarizing the major problem.

- Framework for implementing future code ... and for modelling (even more) complex processes.
- open-source, readily extentable. Encourage help, suggestions, request & improvements to the code.

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- Framework for imp
- open-source, readily

Why Julia ?

- (Very) fast, high-level language (from MIT, since ~ 2012).
- Multiple dispatch ... to distinguish generic code, still dynamic.
- Just in-time (JIT) compilation, fast loops.
- Rapid code development: no linkage; in-built benchmarking.
- Most code & macros are written in Julia.
- Extensive list of packages.
- No storage management, little declaration; type stability.
- Easy documentation.

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Example: Einstein A and B coefficients for the Fe X spectrum;

$$Fe^{9+} \quad [Ne]\ 3s^2\ 3p^5 \rightarrow [Ne]\ 3s\ 3p^6 \ + \ 3s^2\ 3p^4\ 3d$$

```
> wa = Atomic.Computation("Fe X: Einstein",  NuclearModel(36.), ...,
            [Configuration("[Ne] 3s^2 p^5")], ...,
            [Configuration("[Ne ] 3s 3p^6"), Configuration("[Ne] 3s^2 3p^4 3d") ], ...,
            Radiative, Radiative.Settings([M1], [UseCoulomb, UseBabushkin], false, false, ...  )
> perform(wa)

   ... in perform('computation: SCF', ...)
   Compute CI matrix of dimension 1 x 1 for the symmetry 1/2^+ ...   done.
   Compute CI matrix of dimension 1 x 1 for the symmetry 3/2^+ ...   done.
   ...
```

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- Generation of start orbitals
- Computation of angular coefficients (on fly)
- Self-Consistent-Field (SCF) iteration
- Set-up and diagonalization of Hamiltonian matrix
- Breit, QED, many-body corrections, ...

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Example: Einstein A and B coefficients for the Fe X spectrum;

LevI-LevF	I- J / Parity -F		Energy (eV)	Multipol	Gauge	Einstein coefficients A (s^{-1})	gB (m s^{3} J^{-2} s^{-1})	Oscillator strength GF	Decay width (eV)
1 - 2	1/2 +	1/2 -	3.39446D+01	E1	Babushkin	1.35358D+09	7.92148D+18	5.41457D-02	8.90943D-07
1 - 2	1/2 +	1/2 -	3.39446D+01	E1	Coulomb	1.29696D+09	7.59015D+18	5.18810D-02	8.53678D-07
1 - 1	1/2 +	3/2 -	3.58795D+01	E1	Babushkin	2.94707D+09	1.46045D+19	1.05516D-01	1.93980D-06
1 - 1	1/2 +	3/2 -	3.58795D+01	E1	Coulomb	2.65412D+09	1.31527D+19	9.50275D-02	1.74697D-06
2 - 2	1/2 +	1/2 -	4.66937D+01	E1	Babushkin	5.99420D+06	1.34769D+16	1.26717D-04	3.94546D-09
2 - 2	1/2 +	1/2 -	4.66937D+01	E1	Coulomb	7.32071D+06	1.64593D+16	1.54759D-04	4.81858D-09
2 - 1	1/2 +	3/2 -	4.86286D+01	E1	Babushkin	3.51480D+06	6.99614D+15	6.85074D-05	2.31348D-09
2 - 1	1/2 +	3/2 -	4.86286D+01	E1	Coulomb	4.20990D+06	8.37972D+15	8.20557D-05	2.77101D-09
3 - 2	1/2 +	1/2 -	5.03941D+01	E1	Babushkin	1.70893D+08	3.05647D+17	3.10161D-03	1.12484D-07
3 - 2	1/2 +	1/2 -	5.03941D+01	E1	Coulomb	1.81643D+08	3.24872D+17	3.29670D-03	1.19559D-07
4 - 2	1/2 +	1/2 -	5.23240D+01	E1	Babushkin	5.07869D+07	8.11489D+16	8.55010D-04	3.34286D-08
4 - 2	1/2 +	1/2 -	5.23240D+01	E1	Coulomb	5.80616D+07	9.27726D+16	9.77480D-04	3.82168D-08

Jena's Atomic Calculator (JAC)

-- currently supports six types of computations

JAC ... Jena's atomic calculator provides tools for performing atomic (structure) calculations at various degrees of complexity and sophistication. ... JAC also facilitates interactive computations, the simulation of atomic cascades, the time-evolution of statistical tensors as well as various semi-empirical estimates of atomic properties. In addition, the Jac module supports the graphical representation of level energies, electron and photon spectra, radial orbitals and others.

Types of computations:

- Atomic computations of amplitudes, properties and processes.
  ... based on explicitly specified levels and/or electron configurations; many-electron ampltiudes from a given list of (level) properties and atomic processes.
- Complete active-space computations (CAS).
  ... systematic enlargement of the CSF basis due to virtual excitations from reference conf.
- Interactive computations
  ... making use of JAC's high-level atomic language.
- Simulation of atomic cascades following inner-shell excitations.
- Time evolution of statistical tensors in (intense) light pulses.
- Semi-empirical estimates of atomic properties, cross sections, etc.
  ... Lotz formula, asymptotic behaviour of cross sections, etc.

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Not yet implemented (fully); external help & contributions are very welcome.

1 Atomic properties in JAC

– not just level energies and wave functions

Apart from approximate level energies and eigenvectors, JAC supports the computation of the following (level) properties:

+ Einstein ... Einstein A, B coefficients and oscillator strength, without orbital relaxation and for a quick overview of the transition probabilities.
+ HFS ... Hyperfine A and B parameters.
+ IJF_Expansion ... Expansion of atomic states within a IJF-coupled basis.
+ Isotope ... Isotope shift M and F parameters.
+ LandeJ ... Lande g_J factors.
+ LandeF ... Lande g_F factors.
+ Plasma ... CI computations including interactions from various plasma models.
+ Zeeman ... Zeeman splitting of fine-structure levels.

+ Polarizibility ... static and dynamic polarizibilities.
+ Hyperpolar ... hyper-polarizibilities.
+ Stark ... Stark splittings in an external el
+ qZeeman ... quadratic Zeeman splitting.

Not yet implemented.

2 Atomic amplitudes in JAC

– not just level energies and wave functions

Apart from approximate level energies and eigenvectors, JAC will likely support the computation of the following (transition) amplitudes:

+ Anapole ... amplitude of the anapole moment between two (bound-state) levels
+ DipoleZ ... dipole (Stark) operator D_z
+ EDM ... electron EDM interactions
+ MQM ... (electron) magnetic quadrupole moment interactions
+ PNC ... spin-dependent weak interaction
+ PSS ... pseudoscalar-scalar interaction
+ Schiff ... Schiff moment interactions
+ TPT ... tensor-pseudotensor interactions.

Not yet implemented.

3 Atomic processes in JAC

– combining often (bound) levels with a different No. of electrons

In addition, the computation of the following excitation, ionization and decay processes is supported for atoms and ions with N electrons:

+ Auger ... Auger transitions, i.e. the autoionization or emission of a (free) electron into the continuum; $|i(N)> \rightarrow |f(N-1)> + e_A$.
+ dielectronic/DR ... di-electronic recombination, i.e. the dielectronic capture of a free electron and the subsequent emission of photons; $|i(N)> + e \rightarrow |m(N+1)> \rightarrow |f(N+1)> + h\omega$.
+ double Auger ... simultaneous double autoionization cross sections; $|i(N)> \rightarrow |f(N-2)> + e_{A1} + e_{A2}$.
+ impact-excitation ... electron-impact excitation cross sections and collision strengths; $|i(N)> + e \rightarrow |f(N)> + e'$.

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```
+ impact-excitation-autoion/EA   ... electron-impact excitation/autoioniz. cross sections; |i(N)> + e --> |m(N)> + e' --> |f(N-1)> + e' + e_A.
+ impact-ionization/EII          ... electron-impact ionization cross sections; |i(N)> + e --> |f(N-1)> + e' + e_i.
+ multi-photon de-excitation     ... multi-photon excitation and decay amplitudes and cross sections; |i(N)> + n*omega --> |f(N)> or
                                     |i(N)> --> |f(N)> + n*omega.
+ multi-photon ionization        ... multi-photon ionization; |i(N)> + n*omega --> |f(N-1)> + e_p.
+ multi-photon double-ionization ... multi-photon double-ionization; |i(N)> + n*omega --> |f(N-2)> + e_p1 + e_p2.
+ pair-production/PEPP           ... positron-bound-electron pair-production by single-photon absorption; |i(N)> + omega --> |f(N+1)> + e^+.
+ pair-annihilation/PEPASE       ... positron-bound-electron pair-annihilation with single-photon emission: |i(N)> + e^+ --> |f(N-1)> + omega;
                                     cf. PairAnnihlation1Photon.
+ pair-annihilation/PEPATE       ... positron-bound-electron pair-annihilation with two-photon emission:
                                     |i(N)> + e^+ --> |f(N-1)> + omega + omega'; cf. PairAnnihlation2Photon.
+ photo-excitation               ... photon-impact excitation cross sections; |i(N)> + omega --> |f(N)>.
+ photo-excitation-autoioniz.    ... photon-impact excitation-autoionization cross sections; |i(N)> + omega --> |n(N)> --> |f(N-1)> + e_A.
+ photoionization                ... Photoionization processes, i.e. the emission of a single free electron into the continuum due
                                     to an external light field.; |i(N)> + omega --> |f(N-1)> + e_p.
+ radiative                      ... Radiative (multipole) transitions between bound-state levels of the same charge state;
                                     |i(N)> --> |f(N)>  + omega.
+ radiative Auger                ... simultaneous photon emission and autoionization cross sections; |i(N)> --> |f(N-1)> + e_A + omega.
+ radiative-capture/REC          ... radiative electron capture, i.e. the capture of a free electron under the simultaneous emission
                                     of a photon; |i(N)> + e --> |f(N+1)> + omega.
+ Rayleight/Compton              ... elastic and inelastic photon scattering cross sections; |i(N)> + omega --> |f(N)> + omega'.
+ REDA                           ... resonant excitation/electron capture and sequential-double autoionization;
                                     |i(N)> + e --> |m(N+1)> --> |n(N+1)> + e_A1 --> |f(N-1)> + e_A2.
+ READI                          ... resonant-excitation/electron capture auto-double ionization;
                                     |i(N)> + e --> |m(N+1)> --> |f(N-1)> + (e_A1 + e_A2).
```

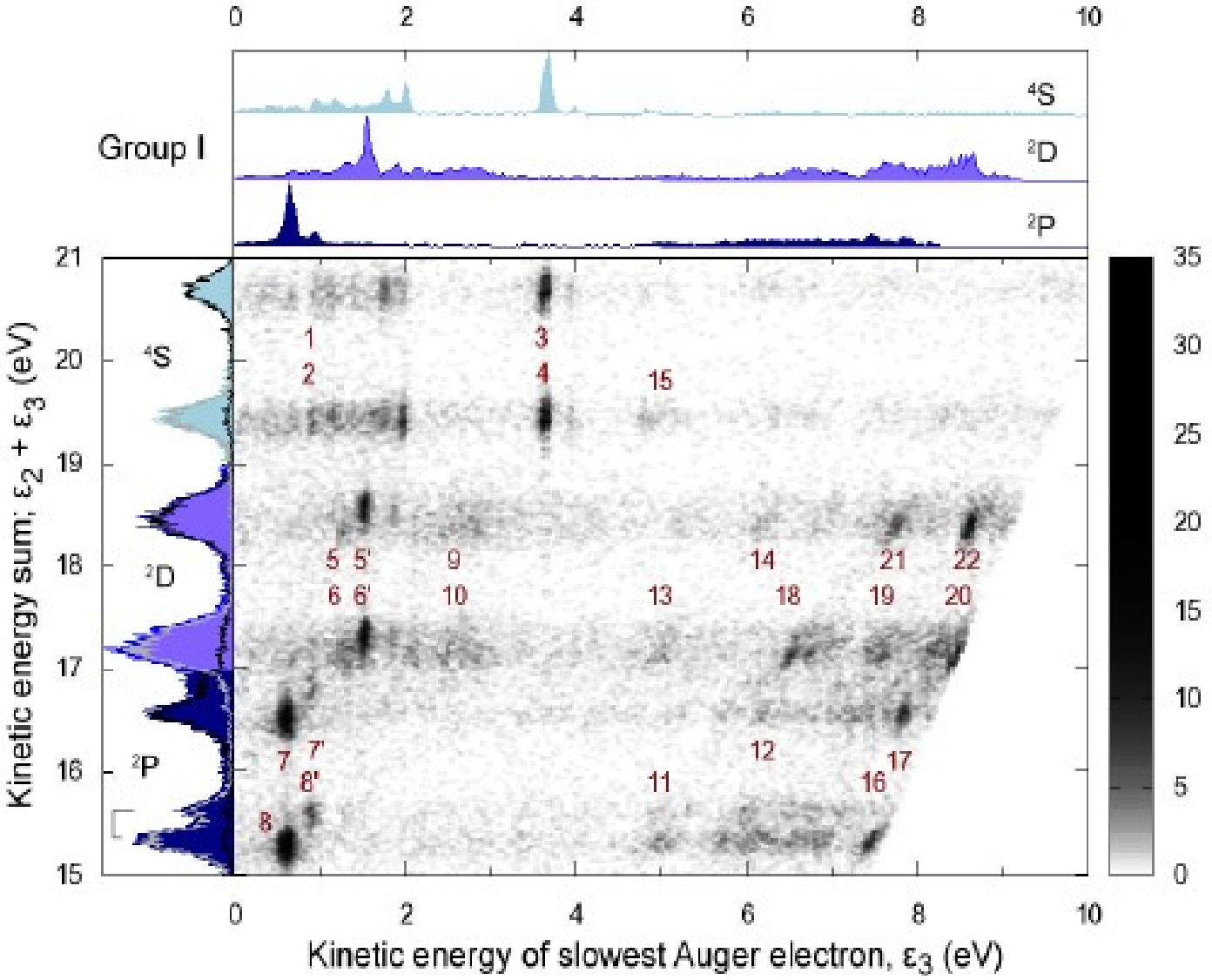
4 Atomic cascades in JAC

– coincidence techniques using a magnetic bottle

$Kr \rightarrow Kr^{3+}$

Double Auger decay of 3d-ionized krypton

- Coincidence on 3d photo electron as first arrival electron.
- Six stripes arise from combination of 3d hole states and the ^4S, ^2D and ^2P finals states of Kr^{3+} $4p^{-3}$
- Dark spots refer to Auger lines.



E. Andersson et al, PRA 82 (2010) 043418.

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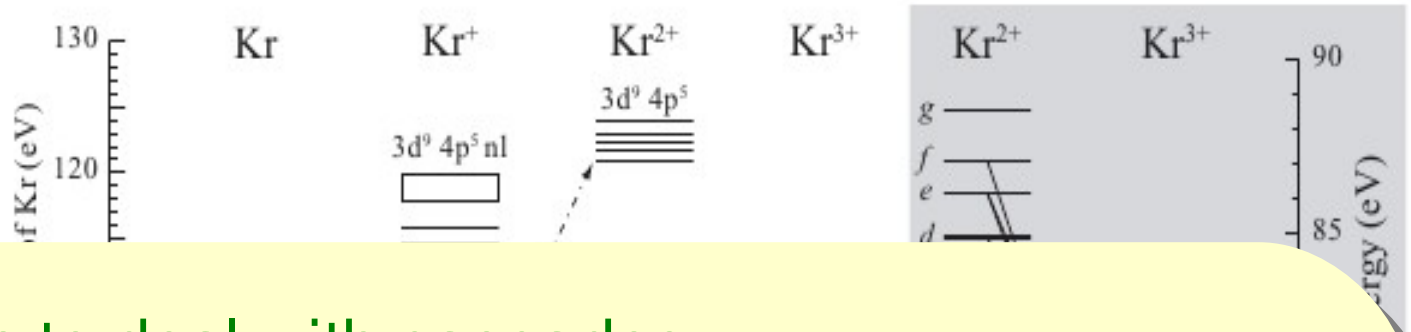

Four approaches to deal with cascades:

- Average singe-configuration approach (averageSCA).

  … 'common set of orbitals' for all ionization stage; 'configuration-averaged' data throughout all simulations

- Singe-configuration approach (SCA).

  … all fine-structure transitions amplitudes are calculated explicitly; still simplified continuum.

- Multiple-configuration approach (MCA).
- Multiple-configuration-shake approach (shakeMCA)

  … incorporates e-e correlations by configuration mixing & shake-transitions.

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- Time evolution o
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  - ... Lotz formula, asymp

JAC as open-source

- Sizeable project: ~ 900 functions/methods, > 25,000 lines
- Improve inline and web documentation.
- Further tests & tutorials.
- Jac on git/Github
- Needs a proper reference.
- Welcomes support & collaboration.

Summary and outlook

- Accurate atomic data are needed (more or less urgently) for a wide range of applications.
- New experimental facilities require an accurate but still simple handling of (a large number of) levels and amplitudes of different kinds.
- In particular, interest in (detailed) analysis of decay cascades, both after inner-shell excitation and in intense light/FEL pulses .
- Stepwise model is – so far – often in good agreement with the observed (photon & electron) spectra; angular distributions and correlations will reveal details of quantum dynamics.

- Present challenge for theory: Improved treatment of open-shell structures and coupling of bound-state densities to the continuum.
- Two (and more-) electron continuum; higher-order processes.
- Interaction with twisted light, tomography of the light-atom interactions, ...